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The Crystal Structure of Nickel Salicylaldoxime

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The structure of nickel salicylaldoxime has been studied by X-ray single crystal methods. The unit cell is monoclinic, space group $P2_1/n$, two molecules per unit cell, and a = 13.63 Å, b = 4.89 Å, c = 10.2 Å, β = 110°26'. The nickel atoms are required to be at symmetry centers and the bonds around the nickel atom must be in a trans planar arrangement. The whole molecule is planar. There appears to be a very strong, short hydrogen bond (2.45 Å) between the phenolic oxygen atom of one organic residue and the oxime oxygen atom of the second organic residue in each molecule.

1. Introduction

This laboratory has been investigating the structures of chelate complexes of analytical importance for the past few years. One of the substances used for the precipitation of nickel is salicylaldoxime (Ephraim 1931). A preliminary investigation of the structure of nickel salicylaldoxime was made by Cox (1935), who showed the crystals to be monoclinic, space group, $P2_1/n - C_{2h}^5$; a = 13.63 Å, b = 4.89 Å, c = 10.20 Å, β = 110°30' and Z = 2. Since the nickel atoms must be at symmetry centers and the molecules must be centrosymmetrical, this substance was selected for further study because of the ease of determination and, furthermore, the comparison of this structure and that of nickel dimethylglyoxime (Godycki and Rundle, 1951, 1953) might be interesting.

2. Experimental

The salicylaldoxime used was an Eastman Kodak Co. product, mp. 56.5-57.5°C with a slight tan color. Its nickel salt was formed according to the method employed by Cox (1935). The green precipitate was filtered, washed with cold water, sucked dry on a Buchner funnel and allowed to dry overnight in the air. Single crystals were grown by dissolving some precipitate in boiling chloroform, allowing the chloroform to cool and then to evaporate slowly at room temperature. Small plates with an average size of about 1.5 x 1.0 x 0.5 mm. result. Small, needle-like crystals with a nearly uniform diameter of about 0.5 mm. were selected for X-ray work. The unit cell dimensions, measured from rotation photographs about the principal axes, were

$$a = 13.63,\ b = 4.88,\ c = 10.2\ \text{Å}$$
$$\beta = 110°26' \text{ (by method of } \omega \text{ separations)}.$$

These values are in good agreement with those reported by Cox (1935). The space group is uniquely determined by the systematic extinctions to be $P2_1/n$ (Cox (1935)

reported $P2_1/m$ apparently due to a typographical error). The observed density of g.cm^{-3} indicates two molecules per unit cell, calculated density = g. cm^{-3}. The molecules must be centrosymmetrical with nickel atoms at symmetry centers.

Multiple-film equi-inclination Weissenberg photographs were taken about [010] for layers n = 0 to n = 3 and about [001] for layers n = 0 to n = 5. Altogether 1097 reflections of measurable intensity were observed and, in addition, 200 reflections were observed to be absent either due to systematic space-group extinctions or to the fact that they were too weak to be recorded. Intensities were estimated visually by comparison with an intensity strip prepared by a series of timed exposures of a typical reflection. A film factor of 3.7 was used. Intensities were corrected in the usual manner for Lorentz and polarization factors and for oblique penetration of the film by the X-rays and the time factor for reflections on non-equatorial layers. All intensities were reduced to a common level by cross-comparison of reflections common to pairs of films. No corrections were made for crystal absorption and the experimental error from this omission may account for a large part of the final discrepancy between observed and calculated structure factors.

3. The Structure Determination

Since the nickel atoms are located at symmetry centers (000 and 1/2, 1/2, 1/2) most reflections of the type (h0l) should have positive structure factors, especially if F is large. One can start immediately with an electron density projection upon (010) using about 142 (h0l) reflections which have F values larger than 5 and assigning these structure factors positive signs. Actually we prepared a Patterson projection upon (010) and calculated structure factors for the reflections from the positions of the atoms read from this Patterson projection. The Patterson shows quite clearly a picture of the molecule. After each electron-density projection, the centers of the atoms were determined by the method of Carpenter and Donohue (1950). New structure factors were calculated and the least-squares-best values of k, the scale factor, and B, the coefficient in the exponent of the isotropic temperature factor in equation (1), were determined.

$$kF_o = |F_c| \exp\left(-B \frac{\sin^2 \theta}{\lambda^2}\right) \qquad (1)$$

The atomic scattering factors used in structure factor calculations were taken from the Internationale Tabellen (1935) with corrections for nickel for the dispersion due to the K electrons with copper Kα radiation being applied according to the formulas of Hönl (1933).

After the fourth electron density projection upon (010) there were no further sign changes in the structure factors and this method of refinement was discontinued. The value of R, defined in equation (2) was,

$$R = \frac{\sum \left(kF_o - |F_c| \exp\left(-\frac{B \sin^2\theta}{\lambda^2}\right) \right)}{\sum kF_o} \qquad (2)$$

however, still 0.24 using all 164 observable reflections of the type (h0l). Figure 1 shows the fourth electron-density projection upon the (010) plane.

With the x and z parameters of the atoms now fairly well established, it was necessary to find the y parameters. A first approximation was obtained by noting that the projected bond lengths parallel to [100] were much shorter than the accepted values for the bond lengths while the projected lengths of bonds perpendicular to [100] were about normal. Using Pauling's (1948) values of bond lengths, the average angle of tilt was about 49 1/4° about an axis lying in the (010) plane and making an angle of 39 1/2° with [001] in obtuse β. Assuming that the molecule was planar and was tilted in this manner, it was possible to calculate approximate values of the y parameters of the atoms.

Structure factors were then calculated for the 1097 observed reflections. The value of R, defined above, was 0.47 at this point. Three bounded electron-density projections for the matter in the region x = 0 to a, y = 0 to b and z = 0 to 0.5c reduced R to only 0.33 for the 450 reflections employed. A three-dimensional electron-density synthesis was calculated for thirteen sections parallel to (010). The intervals chosen were x = 0 to $\frac{a}{2}$ by sixtieths, z = 0 to c by sixtieths and y = 0,1,2,3,4,5,6,7,8,10,11,12 and 14 thirtieths of b.

Centers of atoms were again calculated by the method of Carpenter and Donohue (1950); structure factors were calculated and a least-squares-best value of k and B were obtained. The value of R for all 1097 observed reflections was 0.32 while R for only the (h01) reflections was 0.22 showing that the greatest errors were in the y parameters.

The y parameters were refined by one application of the method of least-squares as developed by Hughes (1941) using the relationship

$$\Delta y_i = \frac{\sum (Fo-Fc)\frac{\partial Fc}{\partial y_i}}{\sum \left(\frac{\partial Fc}{\partial y_i}\right)^2} \qquad (3)$$

Reflections whose signs of Fc were uncertain were given weights of 0 and all others were weighted 1 in this approximation. R was reduced to 0.27 by this refinement, including all 1297 reflections whether observed or not. In the case of an unobserved reflection, F_o-F_c was taken as zero if F_c was less than half the minimum observable value for that region of the film and otherwise it was taken as $1/2\ F_{min} - F_c$ where $F_{min.}$ is the minimum observable value for that region of the film.

The least-squares refinement was applied to all parameters and, after calculating new structure factors and k and β values, R fell to 0.24 for all 1297 reflections and was 0.19 for the (h01) reflections. A further refinement of the y parameters only, by the method of least-squares brought no improvement and only slight shifts of the atomic positions.

An attempt to apply an anisotropic temperature factor was unsuccessful; however, the direction of maximum vibration may not have been properly selected. The structure determination was concluded at this point; further refinements have recently been initiated under a new contract with another agency. Values of the parameters of the atoms are given in Table I.

Table I

Atomic parameters in nickel salicylaldoxime

Atom	x/a	y/b	z/c
Ni	0.500	0.500	0.500
O_2	0.592	0.760	0.503
C_3	0.593	0.935	0.398
C_4	0.680	1.105	0.428
C_5	0.680	1.293	0.318
C_6	0.601	1.299	0.189
C_7	0.513	1.137	0.162
C_8	0.510	0.970	0.270
C_9	0.421	0.787	0.237
N_{10}	0.407	0.585	0.322
O_{11}	0.317	0.442	0.267

Interatomic distances and angles are given in Table II.

Table II

Interatomic Distances and Angles in Nickel Salicylaldoxime

Bonded Atoms		Non-bonded atoms	
Bon	d, Å	Atoms	d, Å
Ni-C_2	1.77	O_2-O_{11}	2.45
Ni-N_{10}	1.87		
O_2-C_3	1.37		
C_3-C_4	1.39		
C_3-C_8	1.41		
C_4-C_5	1.45		
C_5-C_6	1.43		
C_6-C_7	1.38		
C_7-C_8	1.38		
C_8-C_9	1.44		
C_9-N_{10}	1.37		
N_{10}-O_{11}	1.36		

Atoms	Angle	Atoms	Angle
O_2-Ni-N_{10}	95° 12'	C_4-C_3-C_8	118° 35'
$O_2{}^1$-Ni-N_{10}	84° 48'	C_3-C_8-C_7	124° 59'
Ni-N_{10}-O_{11}	120°	C_8-C_7-C_6	116° 30'
C_9-N_{10}-O_{11}	114° 24'	C_7-C_6-C_5	119° 39'
Ni-N_{10}-C_9	125° 15'	C_6-C_5-C_4	121° 27'
N_{10}-C_9-C_8	126° 11'	C_5-C_4-C_3	116° 03'
C_9-C_8-C_3	118° 41'		
C_6-C_2-O_2	125° 09'		
C_3-O_2-Ni	129° 20'		

All atoms of the molecule lie nearly on a plane. The equation of the least-squares best plane in terms of the unit-cell vectors is

$$x + 1.070y - 0.811z = 0$$

Distances of the atoms from this plane vary from zero to 0.10 Å with an average value of 0.04 Å.

Table III gives values of F_o and F_c for all reflections. The value of B, the coefficient in the exponent of the temperature factor is 2.14×10^{-16} cm^2.

4. Discussion of Structure

Several factors contribute to the fairly large value of R, 0.24, which remains in this structure determination. First of all, there is probably an anisotropic temperature factor. It was thought that there should be a direction of minimum vibration in the unit cell about in the $[40\bar{3}]$ direction. This is roughly an axis common to both molecules in the unit cell. However, an attempt to improve R by applying an anisotropic temperature factor, with coefficients determined by the method of least-squares did not cause significant improvement. Another factor causing R to be larger than usual is that we include all reflections even though some are obviously affected by secondary extinction. In the case of unobserved reflections we have included the difference between F_c and $\frac{F\ min}{2}$ whenever F_c is larger than $\frac{F\ min.}{2}$. A third factor is that the scattering due to the hydrogen atoms has been neglected entirely.

Several facts indicate that the structure is reasonably correct in spite of the value of R. The average length of the benzene ring bonds is 1.41 Å, which is in good agreement with the generally accepted value of 1.39 to 1.40 Å. The benzene ring bonds vary in this determination from 1.38 to 1.45 Å. The molecule turns out to be nearly planar with no atom more than 0.10 Å from the least-squares best plane.

Infrared measurements, carried out by Mr. Jack Young under another project, indicate an $O_2{}^1$-O_{11} hydrogen bonded distance of 2.47 Å which is in close

agreement with the distance of 2.45 Å calculated from this structure determination.

There is some evidence of resonance in the six-membered ring containing the nickel atom. Each single bond appears to be 0.06 to 0.10 Å shorter than a normal single bond and each double bond appears to be 0.10 Å longer than the normal isolated double bond. Since the true values for the nickel-oxygen and nickel-nitrogen bonds are not precisely known, it cannot be stated definitely that these bonds are shortened. If there really is some resonance in this chelate ring, then some 4d orbitals must be involved.

The short oxygen-oxygen hydrogen bond distance was unexpected. The two oxygen atoms in this complex are bonded differently and are not exactly similar, except for the hydrogen atom, as they are in nickel dimethylglyoxime in which Rundle (1952) believes there is a symmetrical hydrogen bond. It may be that the bond is not symmetrical in this complex although it is very short.

There are no unusually close approaches between atoms of different molecules and thus the crystal must be held together primarily by van der Waal's forces. There is no indication in this complex of nickel-nickel bonding as there is in the nickel dimethylglyoxime crystal (Godycki and Rundle 1953).

Before any conclusions about the distortion of the salicylaldoxime molecule upon formation of the nickel complex can be drawn, the structure of salicylaldoxime must be determined. We hope to work upon this structure in the near future.

Acknowledgments

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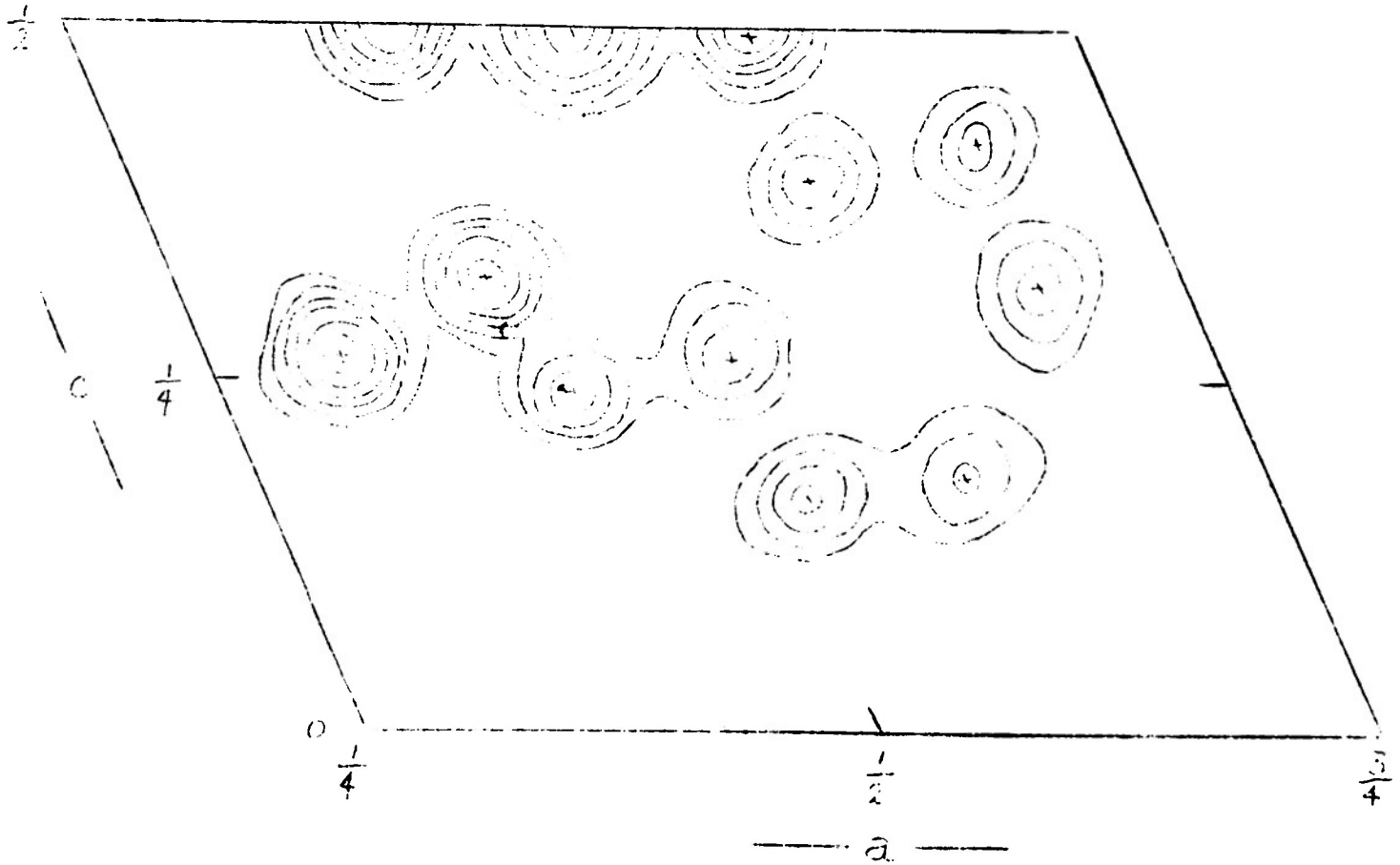

Figure 1. Electron-density projection of one asymmetric unit of nickel salicylaldoxime upon (010). Crosses represent centers of atoms. Contours at 1 e A^{-2} except around nickel atom where contours are at 3,5,10,15, 20 and 25 e. A^{-2}. Outer contour equals 3 e. A^{-2}.

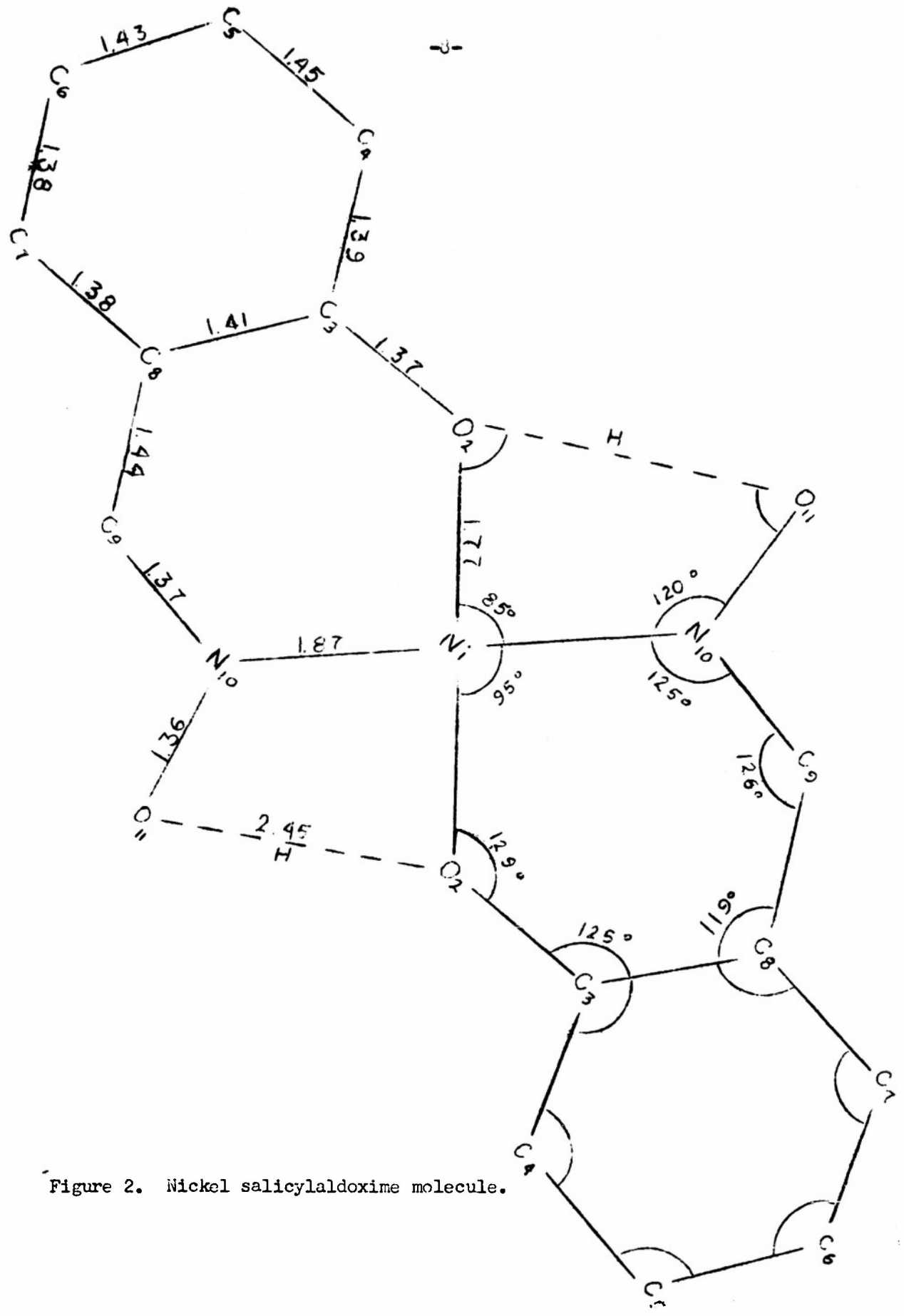

Figure 2. Nickel salicylaldoxime molecule.

Table III

In this table, the reflections are divided into groups of constant "k" and "l" values with regularly increasing values of "h". For each group, the type of reflection is indicated at the beginning, the first column specifies the value of "h", and the second and third columns show the values of F_c and F_o respectively for that reflection. The scale factor applied to the observed structure factors was 1.28, and the value of B in the isotropic temperature factor used in calculating F_c was 2.14.

h 0 0	F_c	F_o
2	83.3	40.0
4	0.0	0.0
6	21.3	23.6
8	4.3	6.7
10	57.3	43.9
12	41.1	38.1
14	1.8	2.6
16	4.4	4.0
h 1 0		
1	21.0	17.3
2	-22.3	23.9
3	- 1.7	4.0
4	4.3	4.6
5	21.4	21.1
6	- 6.0	6.1
7	10.5	10.1
8	- 4.2	2.8
9	8.8	10.0
10	4.4	5.0
11	12.1	14.2
12	5.5	3.3
13	2.7	5.2
14	2.0	2.7
15	4.2	7.0
h 2 0		
0	24.2	31.4
1	- 2.4	2.9
2	22.9	19.5
3	-23.7	29.7
4	43.0	33.3
5	- 6.1	8.4
6	44.0	31.6
7	25.7	19.1
8	20.2	13.8
9	4.8	8.2
10	12.7	14.0
11	- 1.7	3.3
12	8.2	9.2
13	- 2.4	2.4
14	8.3	6.8
15	- 3.3	5.0

h 3 0	F_c	F_o
1	22.2	22.5
2	- 1.8	0.6
3	19.6	19.8
4	-10.9	6.5
5	22.2	21.4
6	5.5	5.8
7	12.4	11.8
8	3.0	3.3
9	7.2	7.4
10	- 3.5	2.8
11	8.8	8.6
12	0.0	0.0
13	9.2	7.0
14	- 2.1	0.8
h 4 0		
0	21.6	18.3
1	9.5	6.9
2	18.1	15.1
3	-12.4	9.1
4	8.4	11.1
5	-12.4	9.7
6	3.9	7.8
7	11.6	7.2
8	9.3	10.0
9	- 2.9	2.9
10	10.8	10.0
11	0.6	2.3
12	7.7	7.0
h 5 0		
1	9.3	10.0
2	8.4	10.5
3	- 2.2	6.1
4	0.0	0.0
5	14.8	16.5
6	2.7	2.7
7	10.3	10.4
8	- 0.4	1.9
9	4.2	5.2

h 6 0	F_c	F_o
0	2.2	3.5
1	- 4.2	4.5
2	7.9	6.8
3	- 3.0	3.1
4	13.4	11.0

h 0 1		
1	83.1	71.9
3	1.7	0.4
5	10.9	15.1
7	10.0	12.4
9	29.9	34.8
11	39.8	35.3
13	16.4	13.1
15	1.7	2.4

h 0 $\bar{1}$		
1	95.0	82.6
3	5.6	4.1
5	12.9	15.5
7	3.7	6.5
9	2.4	5.5
11	22.0	25.7
13	2.4	9.9
15	0.0	0.0
17	0.0	0.0

h 1 1		
0	29.8	22.7
1	11.8	7.5
2	6.6	8.4
3	12.1	11.9
4	42.1	37.2
5	33.8	30.0
6	16.4	16.9
7	- 7.4	6.4
8	21.5	18.8
9	- 5.9	8.6
10	15.8	18.0
11	8.5	4.4

h 1 1	F_c	F_o
12	- 3.4	3.3
13	- 3.8	2.8
14	4.5	5.4
15	3.1	2.0

h 1 $\bar{1}$		
1	- 0.2	2.9
2	82.1	40.2
3	54.6	37.6
4	35.2	31.5
5	-14.8	17.7
6	39.3	37.0
7	-29.4	26.1
8	25.2	24.8
9	- 3.6	2.6
10	9.4	9.1
11	- 2.2	2.7
12	24.0	20.9
13	13.6	10.1
14	18.3	14.7
15	9.8	6.0
16	9.4	8.4
17	0.0	0.0

h 2 1		
0	11.0	10.8
1	7.7	7.9
2	-16.2	15.0
3	34.7	29.2
4	-20.3	15.9
5	41.0	31.9
6	4.6	6.1
7	15.2	12.0
8	- 2.6	3.8
9	21.7	17.5
10	0.0	0.0
11	7.9	9.3
12	0.0	0.0
13	3.9	5.5
14	- 7.0	4.2
15	13.4	3.7

h 2 $\bar{1}$	F_c	F_o
1	46.9	26.9
2	6.0	3.1
3	23.5	25.1
4	9.6	11.4
5	16.0	13.3
6	0.9	3.1
7	30.8	29.1
8	15.4	11.3
9	9.0	11.6
10	- 4.6	3.2
11	14.5	13.6
12	- 6.3	2.4
13	13.2	12.4
14	- 2.4	2.2
15	- 1.6	1.7
16	- 4.7	3.1
h 3 1		
0	20.7	13.7
1	-14.8	21.5
2	- 2.6	2.3
3	-12.3	10.1
4	14.2	12.7
5	14.7	7.2
6	11.5	11.1
7	4.9	4.5
8	15.7	12.2
9	2.2	2.0
10	16.1	13.3
11	- 1.9	2.3
12	2.0	5.8
13	- 3.4	3.9
14	2.9	0.4
h 3 $\bar{1}$		
1	- 8.9	1.9
2	6.4	22.9
3	- 2.4	1.5
4	13.6	11.1
5	-16.0	9.2
6	14.8	12.4
7	5.1	3.7
8	6.8	7.3

h 3 $\bar{1}$	F_c	F_o
9	17.4	11.0
10	4.0	6.1
11	3.4	3.7
12	13.1	10.1
13	- 2.9	1.9
14	6.7	5.4
15	0.0	0.0
h 4 1		
0	- 3.1	3.3
1	20.8	16.6
2	2.8	3.3
3	19.7	19.3
4	2.3	7.6
5	7.7	12.3
6	15.9	13.1
7	7.8	9.5
8	8.5	7.7
9	12.4	14.2
10	- 2.5	2.3
11	9.6	10.2
h 4 $\bar{1}$		
1	20.7	19.6
2	0.0	3.3
3	18.6	16.9
4	-18.6	14.0
5	11.0	10.5
6	- 7.6	8.1
7	14.4	15.4
8	- 3.2	3.3
9	14.1	14.2
10	0.0	0.0
11	7.6	8.7
12	1.4	3.3
13	7.2	3.8

h 5 1	F_c	F_o
0	11.1	10.4
1	4.0	5.1
2	19.6	15.5
3	4.1	2.5
4	11.2	14.2
5	3.3	2.0
6	12.5	12.7
7	- 6.2	5.9
8	- 3.8	2.3
9	-10.7	0.3
h 5 $\bar{1}$		
1	12.3	12.9
2	- 9.9	4.3
3	15.8	12.3
4	9.3	9.3
5	2.4	2.0
6	13.8	15.0
7	2.1	1.8
8	9.3	9.7
9	- 1.6	1.5
10	12.1	9.2
h 6 1		
0	17.0	17.2
1	2.7	1.3
2	0.0	1.2
3	10.8	0.3
4	- 1.0	2.3
h 6 $\bar{1}$		
1	- 2.3	1.5
2	- 6.8	6.5
3	6.1	0.8
h 0 2		
0	-22.5	31.5
2	29.9	31.1

h 0 2	F_c	F_o
4	20.0	2.4
6	10.6	9.9
8	26.0	29.1
10	4.4	5.4
12	2.5	4.6
14	4.4	6.4
h 0 $\bar{2}$		
2	25.5	29.4
4	72.6	50.8
6	1.6	2.3
8	23.2	25.7
10	17.5	19.2
12	6.5	9.0
14	13.5	11.8
16	5.6	5.8
h 1 2		
0	-10.9	9.9
1	3.9	2.8
2	15.6	12.2
3	51.1	35.6
4	32.8	28.8
5	28.7	27.8
6	3.8	9.2
7	38.7	36.6
8	-31.5	24.1
9	35.2	24.1
10	-13.1	11.9
11	3.5	5.5
12	- 4.0	2.9
13	- 8.5	8.8
14	- 6.1	4.7
15	-10.6	6.3
h 1 $\bar{2}$		
1	56.1	36.9
2	76.3	49.3
3	106.0	63.9
4	37.8	34.9
5	31.9	34.7

h 1 $\bar{2}$	F_c	F_o
6	-25.9	28.7
7	30.8	34.7
8	- 9.7	13.3
9	13.9	14.6
10	0.0	0.0
11	4.3	6.3
12	- 8.0	7.8
13	27.5	21.5
14	12.8	10.2
15	14.3	12.5
16	- 3.1	6.3
17	2.8	3.1
h 2 2		
0	9.5	10.0
1	2.2	4.4
2	22.2	20.0
3	12.5	9.9
4	32.2	17.3
5	8.0	9.3
6	9.6	11.0
7	2.5	2.7
8	8.1	11.3
9	2.3	2.4
10	9.3	7.8
11	0.0	0.0
12	8.3	6.8
13	4.0	1.9
14	8.6	7.0
h 2 $\bar{2}$		
1	3.0	1.9
2	22.4	18.7
3	- 7.8	9.5
4	24.6	12.5
5	-13.8	10.5
6	22.2	20.4
7	-12.1	11.0
8	19.5	16.6
9	- 2.5	2.3
10	1.8	4.5
11	1.5	5.1
12	6.4	9.3
13	0.0	0.8
14	5.4	8.2
15	- 4.3	6.3
16	5.6	3.6

h 3 2	F_c	F_o
0	-12.1	9.9
1	22.2	18.8
2	-33.0	19.3
3	20.6	14.2
4	8.0	5.6
5	15.6	10.4
6	1.8	3.7
7	11.4	10.5
8	0.0	0.0
9	12.2	10.5
10	4.2	2.6
11	9.0	7.0
12	-10.8	7.0
13	2.7	4.0
h 3 $\bar{2}$		
1	25.9	20.2
2	-12.5	6.9
3	19.9	15.9
4	3.7	1.5
5	19.8	13.7
6	-14.8	9.0
7	26.5	18.2
8	6.4	2.9
9	19.7	14.1
10	18.2	11.6
11	15.0	12.7
12	- 2.7	2.3
13	9.4	8.7
14	0.0	5.6
15	5.8	3.1
h 4 2		
0	12.9	14.6
1	- 3.8	3.3
2	17.4	19.8
3	8.6	8.8
4	5.8	15.4
5	0.0	0.0
6	- 4.6	5.0
7	- 6.3	6.7
8	12.7	11.2
9	6.0	4.1
10	10.2	12.0

h 4 $\bar{2}$	F_c	F_o
1	- 7.7	7.6
2	17.5	16.6
3	5.5	5.9
4	- 4.6	5.0
5	15.7	14.5
6	- 2.3	7.6
7	- 3.7	3.3
8	12.8	17.0
9	- 1.8	2.9
10	7.1	10.2
11	- 1.7	2.2
12	4.7	7.6
13	1.8	1.4
h 5 2		
0	0.8	2.1
1	19.2	14.3
2	3.8	4.6
3	9.9	12.0
4	11.9	8.3
5	6.0	6.4
6	1.0	1.0
7	8.4	9.5
8	- 6.6	4.2
9	0.0	0.0
h 5 $\bar{2}$		
1	8.3	7.8
2	- 4.1	3.1
3	11.5	11.8
4	3.1	3.3
5	13.1	11.3
6	-11.3	7.3
7	2.8	6.7
8	- 8.9	7.6
9	10.9	11.3
10	1.7	1.7
h 6 2		
0	- 3.4	5.6
1	- 2.7	1.0
2	2.5	0.9
3	- 6.0	5.1
4	0.0	0.0
h 6 $\bar{2}$		
1	- 2.3	6.8
2	5.0	9.2
3	4.0	1.0
4	1.9	0.8
5	- 2.2	7.6

h 0 3	F_c	F_o
1	83.9	72.6
3	52.4	54.3
5	4.1	6.3
7	25.0	24.8
9	5.2	6.5
11	5.1	5.6
13	15.1	16.5
h 0 $\bar{3}$		
1	10.8	17.7
3	45.0	52.4
5	20.1	23.6
7	16.0	27.9
9	58.8	59.9
11	22.3	23.7
13	8.2	8.7
15	10.8	9.6
17	0.9	4.1
h 1 3		
0	9.7	9.8
1	18.0	9.8
2	27.3	27.4
3	15.1	13.2
4	17.0	15.4
5	- 3.6	3.2
6	23.7	24.8
7	- 5.6	8.2
8	26.2	22.1
9	-10.7	10.2
10	11.1	9.9
11	- 2.8	3.2
12	6.7	8.6
13	5.2	6.3
14	6.6	5.5
h 1 $\bar{3}$		
1	6.4	3.6
2	36.7	33.7
3	1.8	1.9
4	47.5	36.6
5	0.6	4.7
6	14.6	17.2
7	- 2.9	3.2
8	18.1	20.0
9	-11.3	12.2
10	7.9	10.8
11	- 5.9	5.2
12	5.7	7.7
13	2.8	2.0
14	13.9	12.4

h 1 $\bar{3}$	F_c	F_o
15	- 4.8	8.1
16	4.6	5.8
17	- 1.0	0.4
h 2 3		
0	-20.1	14.1
1	12.9	10.6
2	17.0	10.4
3	17.5	14.6
4	2.0	2.0
5	29.0	19.3
6	-10.1	8.8
7	24.0	20.9
8	8.8	4.9
9	- 5.6	2.4
10	- 2.9	2.9
11	1.9	3.7
12	1.4	1.9
13	7.1	6.1
h 2 $\bar{3}$		
1	-18.2	11.6
2	0.4	3.5
3	27.0	18.6
4	8.5	5.6
5	60.6	47.2
6	21.6	21.2
7	26.2	25.6
8	-10.4	6.5
9	12.0	13.1
10	2.3	3.0
11	- 1.4	3.5
12	7.2	7.7
13	0.8	5.5
14	2.2	2.8
15	19.1	12.7
16	9.4	4.9
h 3 3		
0	29.1	21.2
1	-10.8	5.0
2	1.0	21.5
3	14.7	4.7
4	19.3	11.4
5	8.7	8.1
6	25.1	17.9
7	- 0.4	3.8
8	12.1	11.6
9	2.4	1.7
10	7.3	7.9
11	- 2.2	2.9
12	13.7	7.8

h 3 $\bar{3}$	F_c	F_o
1	- 3.5	3.8
2	33.6	13.6
3	- 5.7	4.4
4	29.4	22.7
5	- 5.4	6.3
6	19.4	14.5
7	-18.4	10.8
8	12.6	10.6
9	0.4	2.6
10	18.6	14.7
11	1.5	2.7
12	8.6	8.3
13	- 2.9	2.3
14	6.9	5.8
15	0.6	0.8
h 4 3		
0	0.7	3.3
1	12.4	16.0
2	12.1	9.9
3	9.1	12.3
4	3.1	3.3
5	- 2.5	3.5
6	-20.8	19.6
7	- 2.6	2.7
8	- 7.4	8.6
9	8.6	8.7
h 4 $\bar{3}$		
1	20.1	16.9
2	- 0.8	3.3
3	7.9	9.5
4	21.0	5.8
5	- 8.1	3.6
6	9.5	9.9
7	5.8	9.1
8	-12.0	9.2
9	12.5	13.1
10	0.0	1.8
11	12.5	12.3
12	- 0.2	3.3
13	10.9	10.5
h 5 3		
0	13.2	12.4
1	- 1.8	2.6
2	11.6	12.0
3	11.5	10.9
4	3.6	5.9
5	1.5	1.9
6	5.5	6.9

h 5 $\bar{3}$	F_c	F_o
1	2.6	2.9
2	16.1	13.8
3	- 2.4	3.3
4	12.8	12.3
5	2.3	0.9
6	4.0	4.6
7	- 4.9	6.4
8	6.7	10.2
9	- 3.7	3.1
10	8.3	7.7
h 6 $\bar{3}$		
1	12.6	12.4
2	- 0.9	0.8
3	8.6	10.9
h 0 4		
0	63.1	59.2
2	54.3	59.5
4	24.5	33.0
6	12.0	19.1
8	1.9	3.2
10	13.4	12.4
12	21.5	19.3
h 0 $\bar{4}$		
2	1.7	3.7
4	13.4	15.5
6	29.7	34.3
8	24.1	34.7
10	29.4	36.5
12	7.4	10.5
14	4.4	5.0
16	12.2	11.0
h 1 4		
0	12.4	13.1
1	32.6	30.0
2	23.4	24.6
3	14.5	13.1
4	- 4.5	3.2
5	25.3	23.9
6	- 3.9	4.2
7	4.5	9.7
8	7.8	3.7
9	5.9	4.1
10	6.5	2.8
11	13.3	11.5
12	7.0	5.9
13	2.8	4.0

h 1 $\bar{4}$	F_c	F_o
1	29.8	31.7
2	0.1	2.3
3	- 2.2	2.9
4	0.3	3.1
5	30.1	31.7
6	8.2	5.0
7	26.2	29.7
8	-12.7	9.3
9	15.2	17.8
10	- 9.2	8.2
11	19.5	18.4
12	7.8	6.0
13	5.1	7.3
14	4.1	2.9
15	3.0	4.0
16	2.3	6.8
17	8.2	5.1
h 2 4		
0	14.1	12.5
1	10.1	6.9
2	22.8	17.0
3	6.7	4.5
4	27.0	22.4
5	-26.8	16.5
6	41.9	28.5
7	-10.2	8.7
8	12.8	9.9
9	1.4	2.1
10	2.3	2.5
11	- 4.3	1.9
12	4.7	4.5
h 2 $\bar{4}$		
1	9.4	4.9
2	0.3	4.1
3	0.0	0.0
4	51.6	33.5
5	30.3	24.4
6	48.7	62.6
7	9.5	9.9
8	21.6	23.8
9	-21.4	14.8
10	22.3	14.2
11	- 1.1	2.4
12	2.7	5.2
13	- 1.6	2.9
14	7.5	8.2
15	2.8	14.8
16	13.8	8.7

h 3 4	F_c	F_o
0	11.2	9.3
1	20.7	17.4
2	- 0.8	1.8
3	- 1.5	2.2
4	- 6.7	6.4
5	- 2.8	4.2
6	13.1	7.0
7	13.8	11.4
8	3.7	4.5
9	6.2	7.8
10	0.8	2.6
11	8.4	7.9
h 3 $\bar{4}$		
1	14.0	13.2
2	- 2.0	3.2
3	14.2	15.1
4	-14.2	8.7
5	10.6	10.0
6	3.3	2.3
7	-11.2	9.2
8	13.8	10.1
9	4.5	6.4
10	- 4.4	4.4
11	11.4	10.5
12	4.3	3.1
13	3.8	4.7
14	- 1.7	3.1
15	5.7	5.6
h 4 4		
0	28.7	23.3
1	6.3	7.4
2	12.8	10.6
3	1.2	3.3
4	11.7	9.1
5	4.4	2.6
6	3.3	7.3
7	1.9	2.2
8	8.0	8.1
9	- 3.8	3.7
h 4 $\bar{4}$		
1	5.6	5.1
2	29.3	20.4
3	0.9	5.8
4	10.2	11.0
5	- 0.8	3.3
6	13.3	11.6
7	0.0	0.0
8	13.4	9.6
9	- 4.7	2.8

h 4 $\bar{4}$	F_c	F_o
10	13.4	9.6
11	0.9	2.0
12	19.8	12.5
13	2.4	2.3
h 5 4		
0	- 4.2	5.5
1	2.2	4.6
2	3.4	2.2
3	9.8	8.6
4	- 3.6	3.3
5	7.4	10.9
h 5 $\bar{4}$		
1	1.8	3.8
2	2.7	1.8
3	5.8	8.8
4	- 2.7	3.1
5	7.1	9.6
6	4.4	2.2
7	10.5	11.3
8	- 1.6	1.7
9	5.6	5.8
10	0.5	3.2
h 0 5		
1	21.5	27.1
3	13.0	18.2
5	21.9	18.4
7	8.3	5.8
9	13.1	17.7
11	11.6	13.7
h 0 $\bar{5}$		
1	50.1	65.9
3	20.8	30.6
5	28.7	32.6
7	20.1	38.3
9	7.7	15.0
11	21.5	23.4
13	14.5	14.0
15	9.0	7.9
17	11.2	7.4
h 1 5		
0	45.2	47.7
1	0.4	19.3
2	10.5	13.7
3	4.9	4.4

h l 5	F_c	F_o
4	25.3	21.9
5	2.2	3.1
6	5.9	9.6
7	- 7.2	3.6
8	- 1.5	3.3
9	- 5.9	4.2
10	16.9	12.9
11	0.0	0.0
12	7.4	5.8
h l $\bar{5}$		
1	18.1	24.4
2	26.0	29.6
3	29.0	31.9
4	-11.0	9.1
5	4.8	6.5
6	29.0	30.3
7	- 8.6	8.7
8	15.5	19.1
9	- 3.1	2.4
10	16.9	20.7
11	5.4	7.4
12	25.4	23.4
13	11.2	8.7
14	- 0.8	2.6
15	6.1	4.2
16	2.1	2.4
17	- 1.1	0.4
h 2 5		
0	13.6	10.9
1	21.4	15.7
2	7.5	3.6
3	32.7	24.8
4	6.0	3.5
5	23.3	20.6
6	- 3.3	3.3
7	12.4	9.2
8	0.2	2.0
9	9.2	6.4
10	3.7	4.6
11	5.3	4.2
h 2 $\bar{5}$		
1	16.2	16.6
2	-14.2	16.1
3	13.8	17.8
4	- 4.1	4.0
5	20.5	17.4
6	- 5.0	5.1
7	29.2	24.8

h 2 $\bar{5}$	F_c	F_o
8	- 7.7	10.0
9	20.5	18.3
10	- 4.2	2.3
11	9.0	9.9
12	- 6.6	6.3
13	4.8	7.2
14	- 5.9	5.2
15	5.0	6.0
16	0.0	0.0
h 3 5		
0	14.3	24.7
1	4.3	2.3
2	32.5	9.5
3	- 5.4	19.2
4	- 1.2	4.1
5	- 9.2	9.5
6	- 1.0	2.7
7	10.2	4.5
8	7.6	5.8
9	1.3	1.9
10	5.7	4.9
h 3 $\bar{5}$		
1	- 4.0	8.6
2	14.4	16.1
3	- 3.8	6.3
4	12.2	11.5
5	- 7.2	2.2
6	8.5	7.3
7	36.4	26.7
8	16.0	13.6
9	17.8	13.8
10	15.2	14.2
11	-10.9	5.8
12	8.9	7.3
13	- 1.9	1.9
14	8.7	7.8
15	- 5.2	2.3
h 4 5		
0	6.9	6.0
1	11.1	10.1
2	- 0.6	4.4
3	6.8	5.5
4	- 3.9	2.6
5	15.4	9.9
6	6.4	4.0
7	9.4	5.8

h 4 $\bar{5}$	F_c	F_o
1	24.0	18.4
2	6.0	5.4
3	12.8	11.0
4	3.0	3.0
5	13.4	13.3
6	0.0	2.7
7	10.3	10.6
8	1.7	2.7
9	0.0	2.3
10	10.3	7.9
11	8.9	9.0
12	0.9	5.4
13	6.8	5.5
h 5 5		
0	0.2	2.4
1	2.5	1.3
2	4.1	3.6
3	- 2.0	2.3
4	8.1	7.6
h 5 $\bar{5}$		
1	- 0.9	2.3
2	4.0	5.6
3	1.9	2.0
4	13.7	13.3
5	- 2.1	1.9
6	10.5	13.3
7	1.0	1.5
8	4.1	5.2
9	- 0.7	2.0
10	4.3	2.4
h 0 6		
0	26.6	31.3
2	20.4	20.5
4	5.8	12.3
6	9.5	5.5
8	25.9	21.4
10	12.2	13.6
h 0 $\bar{6}$		
2	47.8	58.8
4	17.9	27.9
6	5.9	2.6
8	17.5	25.3
10	20.9	26.5
12	16.0	20.4
14	8.6	10.1
16	4.7	1.9

h 1 6	F_c	F_o
0	7.0	2.7
1	22.0	26.8
2	- 3.2	2.9
3	16.3	18.3
4	7.4	4.9
5	5.6	7.8
6	2.3	2.7
7	2.8	6.8
8	-10.0	7.3
9	12.3	13.7
10	- 3.9	2.3
11	10.1	7.6
h 1 $\bar{6}$		
1	40.5	36.1
2	5.5	7.3
3	21.9	26.4
4	9.7	6.8
5	3.5	12.4
6	- 9.2	11.9
7	21.3	26.2
8	0.0	0.0
9	19.2	22.7
10	- 6.0	4.4
11	24.4	28.9
12	-12.0	6.9
13	18.8	17.0
14	0.0	0.0
15	3.0	4.9
16	0.0	1.5
17	6.5	4.1
h 2 6		
0	- 6.2	1.8
1	-20.3	12.5
2	10.6	7.2
3	- 2.7	4.5
4	19.2	15.0
5	13.8	8.1
6	3.4	5.8
7	1.4	2.9
8	10.4	8.8
9	7.0	4.2
10	4.3	4.1
h 2 $\bar{6}$		
1	- 9.7	7.2
2	24.6	16.4
3	- 2.4	3.2
4	17.1	13.1
5	- 4.4	4.7

h 2 $\bar{6}$	F_c	F_o
6	13.3	11.3
7	- 7.2	8.1
8	15.9	16.0
9	21.1	19.8
10	- 9.1	6.7
11	8.0	9.9
12	3.9	5.9
13	- 3.2	4.0
14	15.3	12.5
15	3.8	1.3
16	5.3	4.9
h 3 6		
0	2.6	2.6
1	14.5	11.8
2	-16.1	11.5
3	28.5	18.3
4	-15.3	8.3
5	13.9	9.7
6	2.3	2.7
7	8.9	5.5
8	6.8	5.0
9	9.9	6.9
h 3 $\bar{6}$		
1	15.3	13.4
2	-10.4	8.7
3	23.0	17.3
4	-13.8	10.0
5	13.9	11.1
6	- 0.1	2.3
7	28.3	27.6
8	15.3	12.7
9	21.8	20.7
10	1.5	2.2
11	7.0	5.9
12	- 4.4	2.6
13	11.7	9.7
14	- 5.7	5.0
15	6.9	4.5
h 0 7		
1	23.5	29.1
3	9.9	15.4
5	14.1	4.7
7	10.9	11.9
9	8.1	13.3
h 0 $\bar{7}$		
1	6.6	15.9
3	30.5	36.4

h 0 $\bar{7}$	F_c	F_o
5	8.7	7.7
7	15.1	11.9
9	24.4	28.4
11	8.2	12.9
13	12.9	15.0
15	11.3	12.8
17	7.4	1.9
h 1 7		
0	23.0	21.4
1	16.1	13.8
2	26.9	24.7
3	1.5	7.0
4	11.0	10.2
5	2.2	2.0
6	15.8	15.5
7	0.0	0.0
8	12.5	8.4
h 1 $\bar{7}$		
1	- 9.5	6.3
2	20.5	22.0
3	3.9	2.8
4	33.4	34.7
5	2.5	2.3
6	18.2	26.6
7	2.5	2.6
8	20.9	26.4
9	- 5.2	7.0
10	21.6	22.3
11	- 8.0	7.3
12	9.1	10.4
13	2.9	2.9
14	10.9	8.2
15	2.3	1.9
16	9.4	6.7
h 2 7		
0	-14.2	8.1
1	- 7.8	2.9
2	-13.3	10.5
3	2.8	3.6
4	5.6	2.4
5	10.6	6.9
6	0.4	2.6
7	15.2	12.5
8	- 2.7	1.5
9	8.5	4.2

h 2 $\bar{7}$	F_c	F_o
1	6.7	6.8
2	1.1	2.7
3	33.1	24.7
4	7.6	3.5
5	24.7	21.1
6	- 7.5	4.1
7	12.7	8.7
8	- 2.6	2.9
9	1.3	3.3
10	11.9	12.4
11	0.7	3.5
12	0.0	0.0
13	15.2	13.2
14	1.9	2.0
15	13.5	9.5
h 3 7		
0	10.4	8.6
1	- 8.1	4.2
2	11.6	13.1
3	35.1	3.8
4	13.0	10.4
5	2.0	1.5
6	7.5	5.2
7	7.2	4.9
8	7.8	4.7
h 3 $\bar{7}$		
1	10.9	2.7
2	17.3	12.7
3	- 7.5	11.1
4	8.9	7.0
5	- 4.3	3.2
6	4.7	4.7
7	4.0	2.3
8	10.8	13.1
9	1.4	2.3
10	7.6	6.1
11	5.9	1.9
12	9.0	6.5
13	- 4.7	3.4
14	6.6	4.7
h 0 8		
0	25.3	20.9
2	11.5	11.6
4	1.0	3.6
6	11.9	8.2
8	10.8	9.7

h 0 $\bar{8}$	F_c	F_o
2	31.0	35.2
4	36.3	37.2
6	6.9	15.1
8	8.3	10.8
10	14.8	17.9
12	18.2	20.2
14	24.5	22.7
16	12.6	10.9
h 1 8		
0	- 5.9	6.4
1	14.9	15.5
2	13.6	9.9
3	8.2	9.5
4	3.6	3.3
5	18.1	15.9
6	0.0	2.8
7	13.8	12.9
h 1 $\bar{8}$		
1	- 1.0	3.3
2	21.6	17.9
3	6.2	9.9
4	1.4	3.3
5	29.6	30.0
6	1.1	3.2
7	8.1	14.3
8	- 9.4	10.1
9	4.6	10.2
10	- 5.2	5.2
11	4.0	4.4
12	18.3	14.7
13	- 5.0	2.8
14	7.1	5.9
15	8.0	6.3
16	- 3.5	1.7
h 2 8		
0	18.1	8.7
1	3.5	2.8
2	6.7	7.3
3	7.6	2.8
4	10.6	7.9
5	4.8	1.7
6	11.1	11.5
h 2 $\bar{8}$		
1	4.7	3.7
2	7.9	6.7

h 2 $\bar{8}$	F_c	F_o
3	0.9	2.2
4	21.3	13.1
5	- 6.1	4.4
6	25.4	14.5
7	- 9.3	6.3
8	12.2	9.9
9	- 5.4	3.6
10	15.1	12.0
11	1.0	3.0
12	9.3	9.0
13	0.9	2.2
14	5.0	5.0
15	- 2.6	0.5

h 3 8		
0	- 3.4	2.6
1	12.2	11.0
2	6.9	5.4
3	2.2	3.5
4	- 1.5	1.9
5	2.2	2.3
6	- 2.2	1.8

h 3 $\bar{8}$		
1	13.5	11.4
2	- 1.7	1.8
3	5.4	5.1
4	- 1.6	2.6
5	6.5	4.7
6	11.3	6.3
7	5.0	5.5
8	- 2.2	2.7
9	12.5	8.6
10	- 2.7	3.5
11	11.4	8.7
12	1.4	1.5
13	5.1	5.1

h 0 9		
1	9.3	15.0
3	12.6	11.6
5	13.6	13.4
7	8.4	5.9

h 0 $\bar{9}$		
1	37.7	37.9
3	24.9	25.6
5	11.3	16.1
7	22.2	26.5
9	9.0	15.1
11	15.9	18.7

h 0 $\bar{9}$	F_c	F_o
13	10.3	15.4
15	0.0	0.0

h 1 9		
0	4.7	4.5
1	5.8	0.4
2	1.4	5.2
3	10.9	8.2
4	9.0	10.6
5	0.0	0.0
6	7.9	8.2
7	0.6	2.3

h 1 $\bar{9}$		
1	15.3	13.2
2	- 3.1	3.6
3	4.0	6.3
4	5.9	9.6
5	0.8	2.0
6	20.3	20.2
7	- 5.2	7.6
8	5.9	10.9
9	-17.6	15.9
10	6.1	7.6
11	1.3	2.9
12	4.5	4.2
13	6.0	5.0
14	1.3	3.5
15	- 1.2	0.5
16	10.4	2.4

h 2 9		
0	2.8	4.4
1	15.0	7.6
2	- 2.1	2.7
3	13.5	6.7
4	- 1.8	1.9
5	14.8	9.7

h 2 $\bar{9}$		
1	9.9	7.0
2	2.5	3.2
3	3.4	5.2
4	- 2.4	2.2
5	19.5	11.1
6	0.4	1.5
7	17.6	13.1
8	8.6	5.8
9	9.5	8.2
10	1.6	2.7

h 2 $\bar{9}$	F_c	F_o
11	11.2	7.7
12	0.7	2.3
13	3.9	3.8
14	0.0	0.0
15	6.8	4.2
h 3 9		
0	8.4	10.4
1	0.0	4.9
2	13.5	4.7
3	- 6.0	1.0
4	7.6	4.6
h 3 $\bar{9}$		
1	- 3.3	1.9
2	15.6	5.5
3	14.7	2.3
4	10.0	7.0
5	3.0	4.0
6	15.8	11.8
7	6.3	4.1
8	8.6	7.6
9	- 4.5	1.9
10	5.6	6.4
11	- 4.0	1.8
12	3.2	3.0
h 0 10		
0	13.9	15.9
2	8.9	12.9
4	13.4	11.6
h 0 $\bar{10}$		
2	10.8	9.1
4	22.3	16.2
6	3.0	4.4
8	19.3	16.9
10	5.9	11.4
12	11.2	10.8
14	9.4	7.3
h 1 10		
0	4.6	4.5
1	9.8	10.1
2	9.1	7.3
3	12.9	12.2
4	3.4	3.7
5	8.0	6.5

h 1 $\bar{10}$	F_c	F_o
1	9.7	11.4
2	- 3.5	3.3
3	12.0	13.2
4	10.9	10.0
5	14.9	15.6
6	10.0	7.4
7	21.8	22.1
8	- 8.0	7.9
9	15.0	16.4
10	- 6.7	4.1
11	10.0	9.1
12	- 2.8	2.4
13	9.7	7.3
14	0.0	0.0
15	8.8	4.4
h 2 10		
0	3.7	4.4
1	- 2.5	1.9
2	7.3	4.5
3	- 9.7	7.9
4	7.3	4.5
h 2 $\bar{10}$		
1	- 9.4	5.8
2	11.6	9.0
3	- 0.4	1.9
4	10.6	6.1
5	2.7	2.8
6	7.2	4.7
7	3.7	4.4
8	7.2	5.2
9	5.6	4.0
10	1.2	3.5
11	- 3.3	4.1
12	4.4	5.2
13	- 4.1	4.9
14	7.7	4.2
h 3 10		
0	0.5	1.5
1	- 1.2	2.3
2	- 2.4	3.1
h 3 $\bar{10}$		
1	3.3	4.7
2	1.3	2.1
3	9.3	7.8
4	0.7	2.0
5	7.5	8.4

h 3 $\bar{10}$	F_c	F_o
6	- 2.4	1.9
7	8.1	6.8
8	3.1	1.9
9	6.0	3.2
10	0.0	0.0
11	3.8	2.9
h 0 11		
1	12.6	16.3
3	6.4	6.4
h 0 $\bar{11}$		
1	35.3	10.6
3	1.8	2.8
5	5.3	3.2
7	6.1	6.1
9	12.5	12.3
11	16.0	18.9
13	10.3	7.6
h 1 11		
0	7.2	6.3
1	0.0	0.0
2	12.8	9.6
h 1 $\bar{11}$		
1	- 2.3	2.3
2	11.3	11.4
3	4.9	2.7
4	17.7	14.8
5	10.0	6.4
6	6.9	9.5
7	- 5.0	4.2
8	10.7	10.0
9	0.9	2.3
10	9.0	7.0
11	4.7	3.7
12	3.1	3.8
h 2 11		
0	6.4	2.4
1	1.9	3.7
h 2 $\bar{11}$		
1	2.1	2.4
2	- 6.2	3.8
3	9.2	7.6
4	1.2	4.0

h 2 $\bar{11}$	F_c	F_o
5	1.4	4.6
6	0.0	0.0
7	7.7	6.9
8	0.0	0.0
9	10.5	7.3
10	0.0	0.0
11	- 0.7	1.8
12	- 6.7	2.9
h 3 $\bar{11}$		
1	0.0	0.0
2	5.2	8.4
3	- 2.1	3.2
4	6.8	5.1
5	0.8	1.9
6	2.9	2.8
7	0.0	0.0
8	10.7	8.6
h 0 12		
0	16.7	17.8
h 0 $\bar{12}$		
2	12.5	13.8
4	13.3	13.2
6	3.7	6.1
8	0.7	2.7
10	16.6	13.7
12	13.9	9.9
h 1 12		
0	- 4.7	3.6
h 1 $\bar{12}$		
1	4.6	4.4
2	0.0	0.0
3	10.9	7.8
4	- 3.7	3.5
5	7.3	4.2
6	-10.5	6.7
7	0.0	0.0
8	- 5.1	2.9
9	5.2	2.7
10	4.4	3.1
11	6.4	3.8

h 2 $\overline{12}$	F_c	F_o
1	0.0	0.0
2	- 0.3	1.0
3	1.3	1.2
4	0.0	0.0
5	- 2.4	5.4
6	0.0	0.0
7	6.5	4.9
8	13.6	9.3
9	5.5	3.7
h 0 $\overline{13}$		
5	8.9	3.5
7	5.4	5.9